Future Directions in Synchrotron Environmental Science at the APS: A Summary of Recent Planning Activities and Recommendations for Future Development

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Our nation, and the world, currently faces the daunting task of characterizing, treating and/or disposing of vast quantities of contaminated materials including high-level nuclear wastes, mining and industrial wastes, atmospheric pollutants, and agricultural pollutants, all of which have major impacts on human health and welfare. To address these problems, both fundamental and targeted studies of complex environmental systems at the molecular level are needed. Synchrotron radiation studies provide the precise information needed to understand these complex systems at the molecular level (see attached bibliography), thereby advancing our knowledge of processes that cannot be otherwise directly studied. The increasingly significant role of synchrotron radiation in the study of environmental systems has led to a rapidly growing field that has become known as "molecular environmental science (MES)".

Adequate resources at the Advanced Photon Source (APS) dedicated to MES research are required to meet current and future demands. The demand for beam time is of two kinds: users conducting individual experiments and established research programs requiring extended access. At the time of this summary, no dedicated stations for MES research existed at the APS, whereas such stations do exist at each of the other DOE-supported synchrotrons.

Planning for future MES research at the APS has taken four forms as summarized below.

"Synchrotron Environmental Science" Workshops: ANL has led the way in developing the synchrotron environmental science community through two workshops (Synchrotron Environmental Science workshops) held at the APS in Spring 1999 (SES-I), and a follow-up workshop (SES-II) held at the APS in Spring, 2002. The SES workshops, attended by up to 150 participants, brought synchrotron scientists together with environmental scientists to explore opportunities for using synchrotron radiation in environmental science research including tutorials to help foster collaborations between the environmental and the synchrotron scientists. SES-III is planned to be held in New York during 2005. The large turnout at these workshops demonstrates the growing interest in MES research.

EnviroSync: EnviroSync (http://envirosync.org; S. Sutton, chair) is a national organization representing the growing community of MES synchrotron radiation users in the U.S.. A recent 60-page EnviroSync report (http://www.slac.stanford.edu/cgi-wrap/getdoc/slac-r-704.pdf) entitled "Molecular Environmental Science: An Assessment of Research Accomplishments, Available Synchrotron Radiation Facilities, and Needs" includes the following recommendations for enhancing US facilities: increased operations support for existing stations, increased station availability and increased support of essential equipment. Station availability increases might be achieved by redirection of existing stations, new stations, and/or enhanced access to innovative instrumentation.

"Future Directions in Synchrotron Environmental Science" Workshop: This workshop, held in conjunction with the 2004 Advanced Photon Source Users Meeting, was the first in a series of workshops on "Future Scientific Directions for the Advanced Photon Source", a study organized by Gopal Shenoy (APS) and Sunil Sinha (UC-San Diego). Invited speakers represented a variety of environmental science endeavors including biogeochemistry, actinide speciation, mineral-water interface processes, contaminant transport, remediation technologies, and analytical instrumentation. Participants agreed that greater recognition of the specialized needs of the environmental science synchrotron user community is needed in large part because environmental samples are among the most demanding of those brought to a synchrotron facility. Additionally, the nature of the samples can vary significantly as do the requirements to handle these samples under carefully controlled environmental conditions. These specialized requirements suggest that science-focused facilities/beamlines should be considered for environmental science research in addition to more distributed resources. The synchrotron user community representing environmental sciences has experienced dramatic growth over the past decade and it is likely that the user base could double over the next decade if dedicated and fully supported facilities are made available to the community.

EnviroCAT: A new sector dedicated to environmental science has been proposed to the APS (S. Sutton, *EnviroCAT* Acting Director). A Letter of Intent was approved by the Program Evaluation Board in 2002. In 2003, a Scientific Proposal was submitted to the Scientific Advisory Committee entitled "Proposal to the Advanced Photon Source Scientific Advisory Committee for an Environmental Science Collaborative Access Team and Sector." The SAC requested a revised proposal with a clearer definition of the biological component of the project and more details and expansion of the sector design. A revised proposal is expected to be submitted to the SAC at its 2005 meeting. The proposed management plan calls for 50% beam time allocation to Institutional Members and 50% to General Users. Thus, half of the project costs would be covered by institutional funds and the other half by a federal grant. *EnviroCAT* currently has three Institutional Members: Argonne National Laboratory – Environmental Research Division, Environmental Protection Agency- National Risk Management Research Laboratory, and the University of Notre Dame. USDA is another potential member as part of the recently approved Multi-State Project entitled "The Chemical and Physical Nature of Particulate Matter Affecting Air, Water and Soil Quality".

Recommendations

A compelling case exists for the development of additional experimental stations for MES research at the APS, primarily focused on microscale techniques, such as microXAFS. This expansion can be accomplished in several ways:

Development of a New Sector: This option is the preferred approach, greatly increasing the amount of dedicated beam time for MES research, maximizing scientific productivity by giving control of the beamline operations to MES scientists and allowing optimization of instrumentation for MES experiments. This option is also the most expensive approach and insufficient monetary support has been identified at this time by the *EnviroCAT* group. Partnering between *EnviroCAT* and the APS in the development of a new sector is an option.

Reassignment of an Existing Sector: This approach will also greatly increase the available beam time dedicated to MES research and at a reduced cost compared to development of a new sector. The trade-off is that any existing sector will not be perfectly suited for MES experiments and substantial upgrading should be anticipated. Existing *EnviroCAT* funding commitments are sufficient to support the operation of an existing sector. Sector 32 is a candidate sector. As above, partnering between *EnviroCAT* and the APS in the operation and upgrade of an existing sector is an option.

Augmentation of an Existing Sector: This option will increase the available beam time for MES research, is the least expensive approach, but will have limited effectiveness. Extensive undulator beam time (required for these brilliance limited experiments) is unavailable for this purpose at existing sectors. In addition, the merging of disparate management styles and scientific programs will lead to inefficiencies and reduced scientific productivity. It should be noted that two of the current *EnviroCAT* institutional members (ANL-ER and U. of Notre Dame) are currently members of MR-CAT (Sector 10), a logical sector where such an augmentation might be pursued.

The APS has a tremendous opportunity to expand its impact on human welfare issues related to environmental challenges. Greatest impact will be realized through the dedication of a full sector operated by MES scientists. Augmentation of existing sectors with new MES programs will be less effective but valuable nonetheless. In all scenarios, the key to success will be the presence of beamline scientists knowledgeable in environmental science problems willing to collaborate with users with broad differences in experience.

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